

# 6,7-Dehydrohyoscyamine

**Inchi:** InChI=1S/C17H21NO3/c1-18-13-7-8-14(18)10-15(9-13)21-17(20)16(11-19)12-5-3-2-4-6-  
**InchiKey:** NZJZSPMNEYIORP-UHFFFAOYSA-N  
**Formula:** C17H21NO3  
**SMILES:** CN1C2C=CC1CC(OC(=O)C(CO)c1cccc1)C2  
**Mol. weight [g/mol]:** 287.35  
**CAS:** 61616-97-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	1.707		Crippen Method
mcvol	223.900	ml/mol	McGowan Method
rinpol	2201.10		NIST Webbook
rinpol	2201.10		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C61616975&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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